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Title: DISCRETE-EXPANSIONS FOR LINEAR INTERPOLATION FUNCTIONS

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Discrete-Expansions for Linear Interpolation Functions

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Abstract

Computational models of particle dynamics often exchange solution data with discretized continuum-fields using interpolation functions. These particle methods require a series expansion of the interpolation function for two purposes: numerical analysis used to establish the model's consistency and accuracy, and logical-coordinate evaluation used to locate particles within a grid. This report presents *discrete-expansions* for two linear interpolation functions commonly used within triangular and tetrahedral cell geometries. Application of the linear discrete-expansions for numerical analysis and localization within particle methods is outlined and discussed.

Discrete-Expansions for Linear Interpolation Functions

Introduction

Particle methods, computational models of particle dynamics, are often solved concurrently with discretized continuum-field equations. Interactive particle methods, including models of liquid sprays, bubble dynamics, and material-interface tracking, strongly couple the governing equations through the bilateral exchange of mass, momentum, and energy. In contrast, reactive particle methods, including models of atmospheric transport, porous-media diffusion, and transient mixing, weakly couple the governing equations; reactive particles simply respond to the entraining continuum field. Another reactive method, used extensively for solution visualization, free-surface tracking, and front tracking, is the tracer-particle method which advects a massless particle with an interpolated velocity. Both interactive and reactive particle methods exchange data with discrete fields using interpolation functions. The focus of this research was on the role of two linear interpolation functions commonly used within particle methods.

Particle methods often use interpolation functions directly to evaluate terms in their governing equations. A Taylor's series of the interpolation function, expanded from the particle's cell, is required to perform analytical studies of these numerical methods. The numerical analyses include establishing the model's mathematical consistency and numerical accuracy. The particle's equations, including kinematic equations-of-motion, are often numerically integrated using multi-step methods such as Runge-Kutta methods. The interpolated quantities that appear within the particle's discretized equations may be evaluated in a neighboring cell, and the required interpolation expansion would then extend through multiple cells in the grid. Derivatives of interpolation functions, however, are generally not continuous across cell boundaries and, therefore, a Taylor's series is not valid in this situation. An alternative expansion for interpolation functions is required to complete numerical analyses for these particle methods.

Particle methods also often use interpolation functions indirectly to evaluate particle-grid connectivity data: the identity of the grid cell in which the particle resides and the particle's logical-coordinate position vector relative to that cell. Particle localization establishes this data using cell-searching and logical-coordinate evaluation methods [1-7]. Cell-searching methods typically use the particle's logical coordinates to both direct and halt the search. Logical-coordinate evaluation involves transforming a physical-space position vector into a local coordinate system, and, as described below, existing methods are based on interpolation expansions. Particle methods, therefore, require the expansion of interpolation functions for numerical analysis and localization, and the mathematical expression required for both purposes is identical; the methods developed herein are, therefore, valid for both purposes.

While multi-cell Taylor's series of interpolation functions are not valid for numerical analyses, modified versions of these expansions are used for particle localization. For spatial-transformation, the arguments of the interpolation function are logical-coordinate and cell-vertex coordinate vectors. Existing logical-coordinate evaluation methods, generalized in Reference [1] for various cell geometries, were developed from a truncated, single-variable Taylor's series expansion of the interpolation function [1,3,5-7]. The modified Taylor's series avoids the problem of discontinuous interpolation derivatives across cell boundaries by ignoring the function's dependence on cell-vertex coordinates. Furthermore, non-linear spatial-transformation problems are linearized by only considering the interpolation function's first-order dependence on logical coordinates. The iterative solution of the resulting system of equations is, however, neither algorithmically robust nor computationally efficient. An alternative expansion for interpolation functions is required for robust and efficient particle localization methods.

An alternative type of expansion, a *discrete-expansion*, was recently proposed and validated for interpolation functions [8-13]. Discrete-expansions are similar to multi-variable Taylor's series, but the new expansions are valid throughout a discretized domain. Discrete-expansions are valid for numerical analyses since they acknowledge the full functional dependence of interpolation and account for discontinuous derivatives across cell boundaries. Furthermore, the solution of discrete-expansions for logical-coordinate evaluation is both algorithmically robust and computationally efficient. Using a simple finite-difference technique, a single discrete-expansion was developed for trilinear interpolation defined within three-dimensional hexahedral cells [8,9]. Multiple discrete-expansions were recently developed for linear and bilinear interpolation functions defined within triangular [12] and quadrilateral cells [13]. These two-dimensional expansions were developed using a total-differential technique [11]. The total-differential development method was also used to obtain discrete-expansions for linear interpolation defined within three-dimensional tetrahedral cells [10].

The purpose of this report is to identify the unique formulations and characteristics of discrete-expansions for linear interpolation. This report will focus on linear interpolation defined within tetrahedral cells; linear interpolation in two-dimensional triangular cells is a simplification of the three-dimensional problem. This report continues by briefly describing the total-differential method of developing discrete-expansions for linear interpolation. Application of the new interpolation expansions for numerical analysis or localization within particle methods is beyond the scope of this report. The utility of linear discrete-expansions for these purposes, however, is outlined and discussed, and then compared to non-linear discrete-expansions.

Linear Interpolation

Three-dimensional computational space is frequently discretized into tetrahedral cells. Linear functions are often applied within these cells for both data interpolation and spatial-transformation. Interpolation produces a continuous mapping of discrete field data, often located at cell-vertices, to any position within the cell. Spatial transformation includes mapping cell geometries from a physical-space, $\bar{X} = (x, y, z)^T$, to a logical-space, $\bar{\xi} = (\xi, \eta, \zeta)^T$, coordinate system; see Figure 1. The linear interpolation function is dependent upon both $\bar{\xi}$ and the cell-vertex (cv) coordinate vector, $\bar{X}^{cv} = ({}^0\bar{X}, {}^1\bar{X}, {}^2\bar{X}, {}^3\bar{X})^T$, as presented in Equation 1.

$$\begin{aligned} \bar{X}(\bar{\xi}, \bar{X}^{cv}) = {} & (1 - \xi - \eta - \zeta)\ {}^0\bar{X} \\ & + (\quad \xi \quad)\ {}^1\bar{X} \\ & + (\quad \eta \quad)\ {}^2\bar{X} \\ & + (\quad \zeta \quad)\ {}^3\bar{X} \end{aligned} \tag{1}$$

Equation 1 is linear with respect to the logical-coordinates, $\bar{\xi}$, and cell-vertex coordinates, $\bar{X}^{cv}$. While the physical coordinates of the tetrahedral's vertices are arbitrary, the transformed coordinates are bound by $\xi \geq 0$, $\eta \geq 0$, $\zeta \geq 0$, and $\xi + \eta + \zeta \leq 1$. Interpolated data fields, produced by the application of Equation 1 throughout the entire domain, are continuous along the common boundaries of adjoining cells. Using Equation 1, linear interpolation within triangles is obtained by setting $\zeta = 0$, and within one-dimensional line-elements by setting $\eta = \zeta = 0$.

Total Differential

Using the interpolation function, $\bar{X}(\bar{\xi}, \bar{X}^{cv})$, the objective is to establish a relationship between the finite change of the physical coordinates, $\Delta\bar{X}$, the logical coordinates, $\Delta\bar{\xi}$, and the cell-vertex coordinates, $\Delta\bar{X}^{cv}$. The function's total-differential provides a relationship between infinitesimal changes of these coordinates, $d\bar{X} = f(d\bar{\xi}, d\bar{X}^{cv})$, as presented in Equation 2.

$$d\bar{X} = \frac{\partial\bar{X}(\bar{\xi}, \bar{X}^{cv})}{\partial\bar{\xi}}\, d\bar{\xi} + \frac{\partial\bar{X}(\bar{\xi}, \bar{X}^{cv})}{\partial\bar{X}^{cv}}\, d\bar{X}^{cv} \tag{2}$$

Equation 2 includes two interpolation derivatives that are scaled by differential coordinate vectors. The first derivative represents a coordinate-transformation or Jacobian matrix: $\partial\bar{X}/\partial\bar{\xi}$. The size of the square Jacobian matrix is equal to the number of spatial dimensions. The second derivative represents a geometry-transformation matrix: $\partial\bar{X}/\partial\bar{X}^{cv}$. The number of rows and columns in this non-square matrix are equal to the dimension size and the number of elements in the cell-vertex coordinate vector. For linear interpolation, the coordinate-transformation matrix is linear with respect to $\bar{X}^{cv}$, and the geometry-transformation matrix is linear with respect to $\bar{\xi}$. The linear interpolation function's simplified total-differential is presented in Equation 3.

$$d\bar{X} = \frac{\partial\bar{X}}{\partial\bar{\xi}}(\bar{X}^{cv})\, d\bar{\xi} + \frac{\partial\bar{X}}{\partial\bar{X}^{cv}}(\bar{\xi})\, d\bar{X}^{cv} \tag{3}$$

Integration Method

The objective is to integrate Equation 3 to obtain a discrete-expansion for interpolation: $\Delta\bar{X} = f(\Delta\bar{\xi}, \Delta\bar{X}^{cv})$. The limits of integration are two particles located in separate, non-contiguous grid cells: State 1, $\bar{X}_1 = \bar{X}(\bar{\xi}_1, \bar{X}_1^{cv})$, and State 2, $\bar{X}_2 = \bar{X}(\bar{\xi}_2, \bar{X}_2^{cv})$. Integration of Equation 3 between two particle end-states is represented in Equation 4.

$$\int_1^2 d\bar{X} = \int_1^2 \frac{\partial\bar{X}}{\partial\bar{\xi}}(\bar{X}^{cv})\, d\bar{\xi} + \int_1^2 \frac{\partial\bar{X}}{\partial\bar{X}^{cv}}(\bar{\xi})\, d\bar{X}^{cv} \tag{4}$$

The linearity of the interpolation derivatives affects the complexity of the solution of Equation 4. More importantly, both $\partial\bar{X}/\partial\bar{\xi}$ and $\partial\bar{X}/\partial\bar{X}^{cv}$ must be continuous for the total-differential to be valid within a specified region. Within a single cell, solution of Equation 4 is straightforward; the interpolation derivatives are guaranteed to be continuous in this region. In contrast, if the limits of integration cross a cell boundary, where interpolation functions are continuous but their derivatives are generally discontinuous, the total-differential is not valid. Discrete-expansions may be obtained from Equation 4 if the integration pathline is partitioned into cell-based line-segments, but this technique is prohibitively complex and expensive.

Parameterization

Alternatively, the coordinate-space between the limits of integration can be parameterized. Parameterization removes the concept of multiple coordinate systems and, thus, discontinuous interpolation derivatives, by creating a single coordinate-space between two particles. The integration pathline end-states can then be defined within any grid cells, including non-contiguous cells. While the form of the parameterization function is arbitrary, it must be differentiable; it is embedded within the parameterized interpolation function. The parameterized interpolation derivatives are then guaranteed to be continuous along the integration pathline. The parameterized total-differential may then be integrated without requiring a partitioned pathline.

To create a single coordinate-space between two particles, each of the physical, logical, and cell-vertex coordinates must be parameterized; particle states are a collection of these vectors. A simple, linear technique using the variable 's', where $0 \le s \le 1$, was selected in this research.

The parameterized coordinates, $\bar{X}(s)$, $\bar{\xi}(s)$ and $\bar{X}^{cv}(s)$, then vary linearly along any integration pathline. Integration limits for the parameterized total-differential are the bounding limits of ‘s’. Integration of the parameterized total-differential is represented in Equation 5.

$$\int_0^1 \frac{\partial \bar{X}(s)}{\partial s}\, ds \;=\; \int_0^1 \frac{\partial \bar{X}}{\partial \bar{\xi}}(\bar{X}^{cv}(s))\, \frac{\partial \bar{\xi}(s)}{\partial s}\, ds \;+\; \int_0^1 \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}(s))\, \frac{\partial \bar{X}^{cv}(s)}{\partial s}\, ds \tag{5}$$

Solution of Equation 5 requires an integration pathline defined between two particles end-states. An integration pathline for the parameterized total-differential traverses through the $(\bar{\xi}, \bar{X}^{cv})$ plane since these vectors are the arguments of the interpolation function as defined for spatial transformation: $\bar{X} = \bar{X}(\bar{\xi}, \bar{X}^{cv})$. The parameterization function, however, does not prescribe the shape of the integration pathline. Three unique integration pathlines were selected by this research to solve Equation 5: direct, upper-step, and lower-step integration pathlines.

Discrete-Expansions

The purpose of this section is to review the discrete-expansions for linear interpolation developed using the total-differential method. Details of this development, including integration of Equation 5, are provided in References [10-13]. At the end of this section, the general form of these expansions will be discussed. The final section will discuss the application of linear discrete-expansions for numerical analysis and localization within particle methods.

Direct Pathline The first integration pathline used to solve Equation 5 is a direct line between States 1 and 2; see Figure 2. The three discrete-expansions for linear interpolation most easily obtained using the direct integration pathline are presented in Equation 6.

$$\begin{aligned}
\Delta\bar{X} &= \frac{\partial \bar{X}}{\partial \bar{\xi}}(\hat{\bar{X}}^{cv})\,\Delta\bar{\xi} && && + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\hat{\bar{\xi}})\,\Delta\bar{X}^{cv} \\
\Delta\bar{X} &= \frac{\partial \bar{X}}{\partial \bar{\xi}}(\bar{X}^{cv}_1)\,\Delta\bar{\xi} &&+ \frac{\partial \bar{X}}{\partial \bar{\xi}}(\Delta\bar{X}^{cv})\,\Delta\bar{\xi} && + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}_1)\,\Delta\bar{X}^{cv} \\
\Delta\bar{X} &= \frac{\partial \bar{X}}{\partial \bar{\xi}}(\bar{X}^{cv}_2)\,\Delta\bar{\xi} &&- \frac{\partial \bar{X}}{\partial \bar{\xi}}(\Delta\bar{X}^{cv})\,\Delta\bar{\xi} && + \frac{\partial \bar{X}}{\partial \bar{X}^{cv}}(\bar{\xi}_2)\,\Delta\bar{X}^{cv}
\end{aligned} \tag{6}$$

Upper-Step Pathline The second integration pathline used to solve Equation 5 is comprised of two line-segments between States 1 and 2. The first pathline segment is a line of constant $\bar{\xi}$ from State 1 to State A; see Figure 2. The second pathline segment is a line of constant $\bar{X}^{cv}$ from State A to State 2. These two pathline segments form an upper-step within the $(\bar{\xi}, \bar{X}^{cv})$

plane. The single discrete-expansion for linear interpolation most easily obtained using the upper-step integration pathline is presented in Equation 7.

$$\Delta\bar{X} \;=\; \frac{\partial\bar{X}}{\partial\bar{\xi}}(\bar{X}_2^{cv})\,\Delta\bar{\xi} \;+\; \frac{\partial\bar{X}}{\partial\bar{X}^{cv}}(\bar{\xi}_1)\,\Delta\bar{X}^{cv} \tag{7}$$

Lower-Step Pathline The third integration pathline used to solve Equation 5 is comprised of two line-segments between States 1 and 2. The first pathline segment is a line of constant $\bar{X}^{cv}$ from State 1 to State B; see Figure 2. The second pathline segment is a line of constant $\bar{\xi}$ from State B to State 2. These two pathline segments form a lower-step within the $(\bar{\xi}, \bar{X}^{cv})$ plane. The single discrete-expansion for linear interpolation most easily obtained using the lower-step integration pathline is presented in Equation 8.

$$\Delta\bar{X} \;=\; \frac{\partial\bar{X}}{\partial\bar{\xi}}(\bar{X}_1^{cv})\,\Delta\bar{\xi} \;+\; \frac{\partial\bar{X}}{\partial\bar{X}^{cv}}(\bar{\xi}_2)\,\Delta\bar{X}^{cv} \tag{8}$$

The five discrete-expansions in Equations 6-8 are similar to a Taylor's series of the linear interpolation function; they are combinations of derivatives scaled by the vectors $\Delta\bar{\xi}$ and $\Delta\bar{X}^{cv}$. These discrete-expansions also have a limited number of terms; for linear interpolation, only first-order derivatives are non-zero. Arguments of the interpolation derivatives include end-state coordinates, the vector $\Delta\bar{X}^{cv}$, and the averages $\hat{\bar{\xi}} = (\bar{\xi}_1 + \bar{\xi}_2)/2$ and $\hat{\bar{X}}^{cv} = (\bar{X}_1^{cv} + \bar{X}_2^{cv})/2$.

The discrete-expansion obtained using the upper-step pathline, Equation 7, is similar to the expansion obtained using the lower-step pathline, Equation 8. Within Equation 7, $\partial\bar{X}/\partial\bar{\xi}$ is evaluated at $\bar{X}_2^{cv}$; the logical-coordinates vary along the pathline segment where $\bar{X}^{cv}$ is fixed at State 2. Similarly, $\partial\bar{X}/\partial\bar{X}^{cv}$ is evaluated at $\bar{\xi}_1$; the cell-vertex coordinates vary along the pathline segment where $\bar{\xi}$ is fixed at State 1. While the form of the lower-step expansion is nearly identical to the upper-step expansion, the interpolation derivatives are evaluated at opposite particle end-states; these integration pathlines are exact mirror images of each other.

The linear discrete-expansions in Equations 6-8 are a simplification of the bilinear [11,13] and trilinear expansions [8,9]; linear interpolation is more simple than a multi-linear function. Furthermore, the total-differential and finite-difference methods produce identical discrete-expansions for similar interpolation functions. The discrete-expansion in Equation 7 is the linear version of the upper-step bilinear expansion. The bilinear discrete-expansion, obtained using the total-differential method, is the two-dimensional version of the trilinear expansion obtained using the finite-difference method; bilinear interpolation is a subset of the trilinear function.

However, unique discrete-expansion formulations are possible for linear interpolation; the transformation matrices are easily manipulated since they are linear functions of $\bar{\xi}$ and $\bar{X}^{cv}$. Two expansions in Equation 6 include transformation matrices that are evaluated at the identical particle end-state. A second Jacobian matrix, evaluated with $\Delta\bar{X}^{cv}$, also appears in these expansions. The form of these two expansions is not repeated in the multi-linear solutions. Furthermore, these direct-pathline expansions are related to the other linear discrete-expansions; they are equivalent to the upper-step and lower-step expansions in Equations 7 and 8.

Discussion

Particle methods require expansions of interpolation functions for numerical analysis and logical-coordinate evaluation. Application of the expansions developed herein for these purposes is beyond the scope of this report. Verification of the new discrete-expansions is provided in References [8-13]. Within the following sections, application of linear discrete-expansions for numerical analysis and localization within particle methods is outlined and discussed.

Numerical Analysis

The goal of numerical analysis, an analytical investigation of a computational model, includes establishing the model's mathematical consistency and numerical accuracy. While estimates of these measures are possible, analytical proof is preferred. A model's consistency and accuracy are based upon its leading-order error term, which is evaluated by substituting series expansions for all discrete-terms within the model. A Taylor's series, however, is not a valid expansion for coupled multi-linear interpolation functions. Instead, a discrete-expansion is required to complete numerical analyses of computational models that use interpolation.

Numerical analyses of reactive particle methods require a discrete-expansion of a velocity-interpolation function; these methods compute particle trajectories by interpolating from a discrete velocity field. All numerical analyses require that the discrete-expansion must be written relative to a single state, defined here as State 1. Using multi-step integration methods, however, a reactive particle's velocity might be evaluated in a separate, non-contiguous grid cell, defined here as State 2. The objective is then to write a discrete-expansion of the velocity-interpolation function from State 1 to State 2: $\bar{V}_2 = \bar{V}_1 + f(\bar{\xi}_1, \bar{V}_1^{cv})$.

Any one of the above discrete-expansions may be used for numerical analysis; each expansion is valid throughout a discretized domain. One obvious choice would be the common expansion obtained using both the finite-difference and total-differential development methods. For linear interpolation, the common discrete-expansion, originally presented in Equation 7, is repeated in Equation 9 for a velocity-interpolation function.

$$\bar{V}(\bar{\xi}_2, \bar{V}_2^{cv}) \;=\; \bar{V}(\bar{\xi}_1, \bar{V}_1^{cv}) \;+\; \frac{\partial\bar{V}}{\partial\bar{\xi}}(\bar{V}_2^{cv})\,\Delta\bar{\xi} \;+\; \frac{\partial\bar{V}}{\partial\bar{V}^{cv}}(\bar{\xi}_1)\,\Delta\bar{V}^{cv} \tag{9}$$

For numerical analysis, discrete-expansions must be defined at a single state, but Equation 9 includes an interpolation derivative defined at State 2: $\partial\bar{V}(\bar{V}_2^{cv})/\partial\bar{\xi}$. Recursive application of the discrete-expansion can transform a mixed-state interpolated velocity into a State 1 function: $\bar{V}(\bar{\xi}_1, \bar{V}_2^{cv}) = f(\bar{V}^{cv}(\bar{\xi}_1, \bar{V}_1^{cv}))$. This separate single-state velocity-interpolation expansion can be substituted into Equation 9, and the model's numerical analysis may then be completed.

For computational models that use interpolation, discrete-expansions represent a key advancement in the ability to analyze existing models; discrete-expansions provide the capacity to analytically evaluate their mathematical consistency and numerical accuracy. By providing an analytical description of a model's leading-order error term, discrete-expansions also provide the capacity to develop advanced computational models; the leading-order error term of an existing model may be used to create a new, advanced computational model.

Logical-Coordinate Evaluation

Logical-coordinate evaluation is the transformation of a physical-space position vector into a cell-based, logical-coordinate system. Interpolation functions are often used for spatial transformation because they can provide a relationship between physical and logical coordinates. Discrete-expansions represent the mathematical expression that allows interpolation functions to evaluate a particle's logical-coordinates. For linear interpolation, the discrete-expansion originally presented in Equation 7 may be rewritten for this purpose as presented in Equation 10.

$$\frac{\partial\bar{X}}{\partial\bar{\xi}}(\bar{X}_2^{cv})\,\Delta\bar{\xi} \;=\; (\bar{X}_2 - \bar{X}_1) - \frac{\partial\bar{X}}{\partial\bar{X}^{cv}}(\bar{\xi}_1)\,\Delta\bar{X}^{cv} \tag{10}$$

Equation 10 is valid between two particles, States 1 and 2, located in separate, non-contiguous grid cells. For logical-coordinate evaluation, the coordinate vectors defined at State 1 are known: $\bar{X}_1$, $\bar{\xi}_1$ and $\bar{X}_1^{cv}$. In contrast, the only coordinates known at State 2 are the physical-coordinates of the particle: $\bar{X}_2$. The cell-searching portion of the localization algorithm does provide cell-vertex coordinates at State 2: $\bar{X}_2^{cv}$. The only unknown in Equation 10 is the logical-coordinate vector at State 2, $\bar{\xi}_2$, which is the desired solution embedded within $\Delta\bar{\xi} = \bar{\xi}_2 - \bar{\xi}_1$.

Equation 10 is defined between two *fixed* particles. State 2 is *absolutely* fixed, invariant throughout the localization problem, by the particle's physical-coordinates, $\bar{X}_2$. In contrast, State 1 is *arbitrarily* fixed; its position is constrained only by the requirement that $\bar{X}_1 = \bar{X}(\bar{\xi}_1, \bar{X}_1^{cv})$. Bound position vectors may then be selected for use in Equation 10 that guarantees an algorithmically robust method. Solution of Equation 10 is also computationally efficient; all of the interpolation derivatives are constant and only require a single evaluation. Furthermore, in contrast to the multi-linear discrete-expansions, only a single solution of Equation 10 is required for logical-coordinate evaluation since elements of $\bar{\xi}_2$ only appear within $\Delta\bar{\xi}$.

Summary

Five new discrete-expansions were developed for linear interpolation as defined within triangular and tetrahedral cells. These expansions were developed by parametrically integrating the interpolation function's total-differential between two particles located within separate, non-contiguous grid cells. Discrete-expansions are similar to multi-variable Taylor's series, but the new expansions are valid throughout a discretized domain. For particle methods, discrete-expansions are valid for numerical analyses since they account for interpolation discontinuities across cell boundaries. The use of discrete-expansions for logical-coordinate evaluation also provides an algorithmically robust and computationally efficient particle localization method.

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Figures

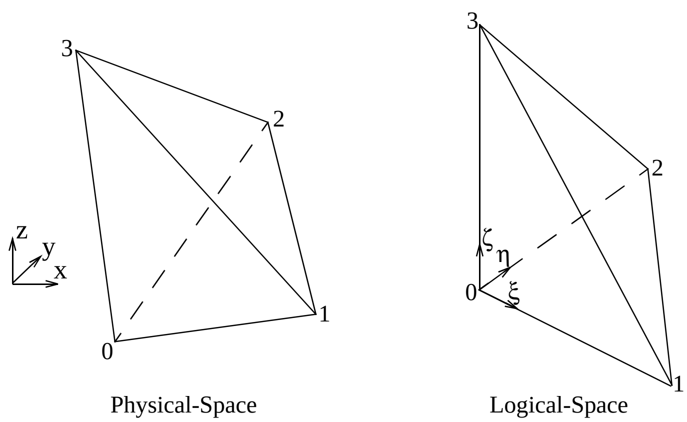

Figure 1: Coordinate Transformation

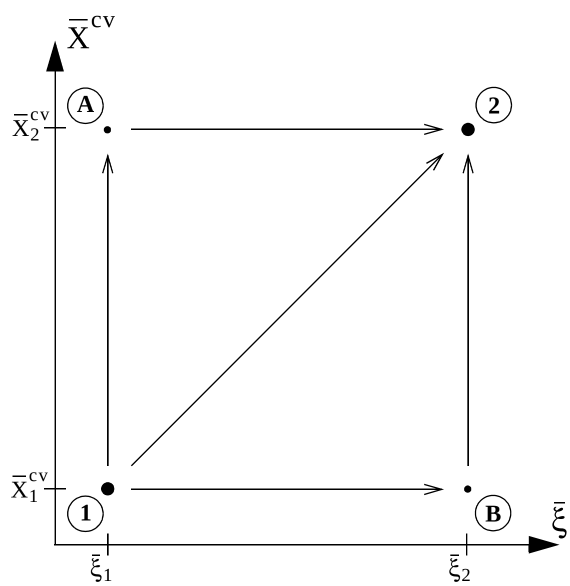

Figure 2: Integration Pathlines